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Office of
Science
U.S. DEPARTMENT OF ENERGY

A U.S. Department of Energy laboratory
managed by UChicago Argonne, LLC

Vis Breakout

Mark Hereld & Joe Insley

ALCF's Eureka and Gadzooks

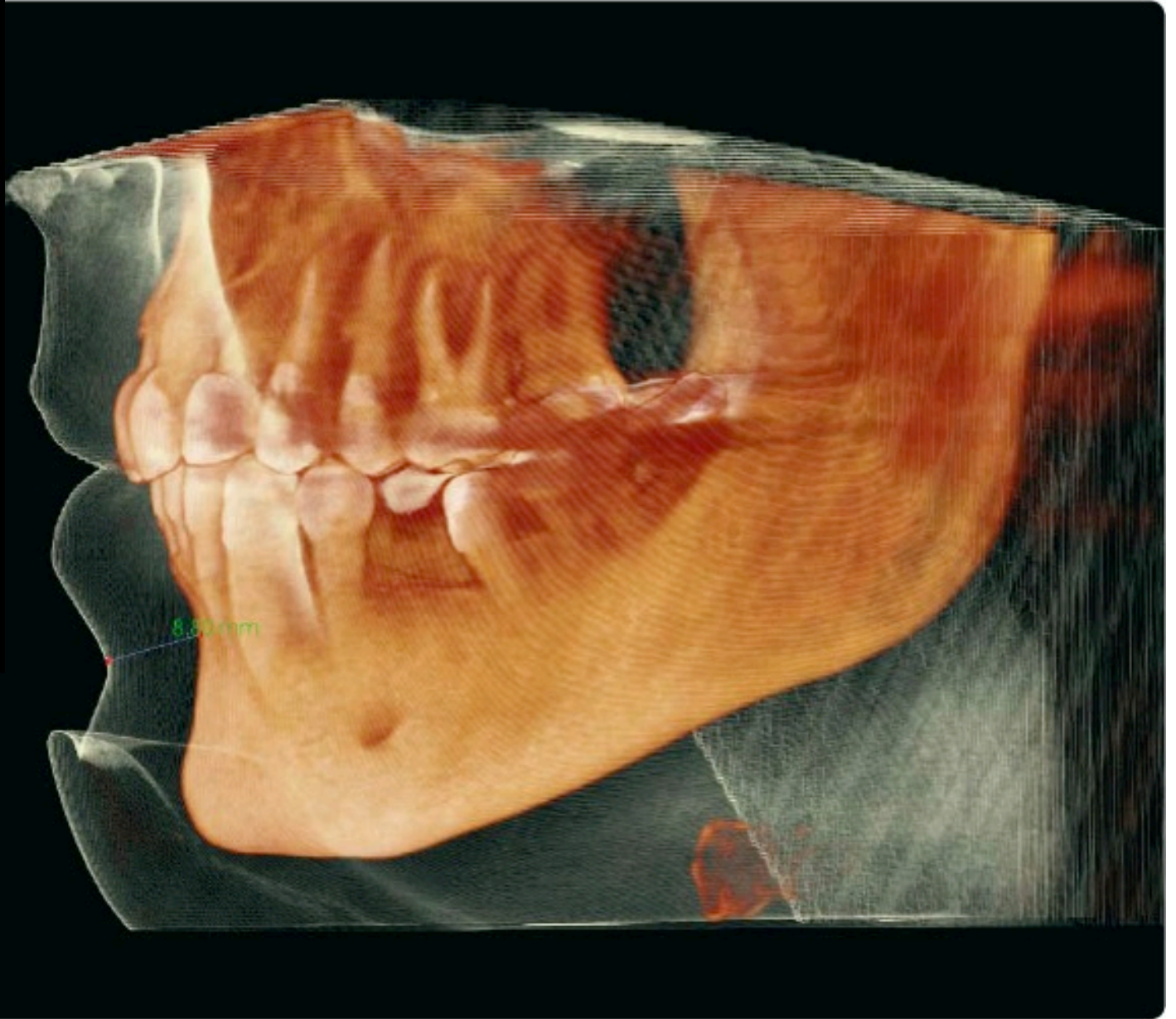
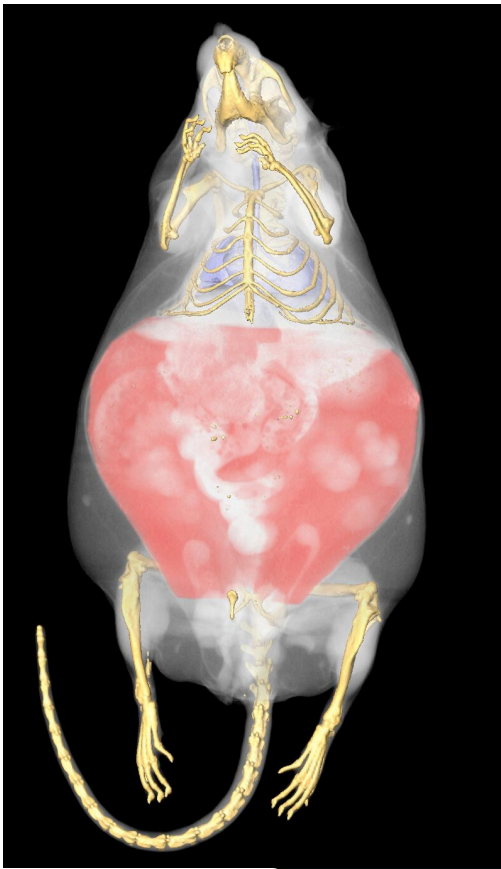
- 104 dual quad core servers
- 208 Quadro FX5600 graphics engines
- 312 Gbytes of total frame buffer RAM
- 3.2 TB of total system RAM
- Each node (server):
 - Dual quad core CPU
 - 2 GPUs
 - 1.5 GB frame buffer RAM
 - 32 GB system RAM

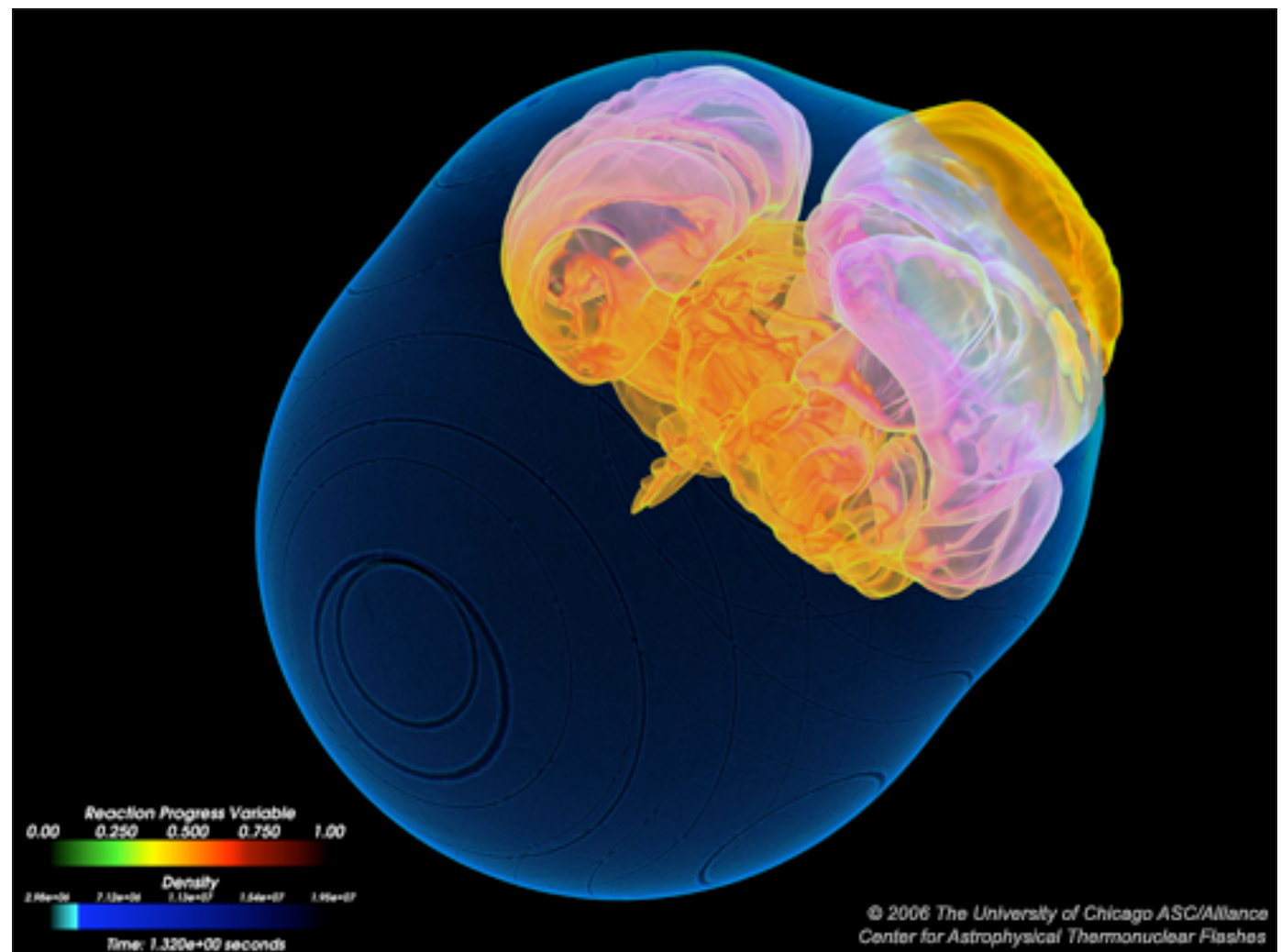
Under the Circumstances

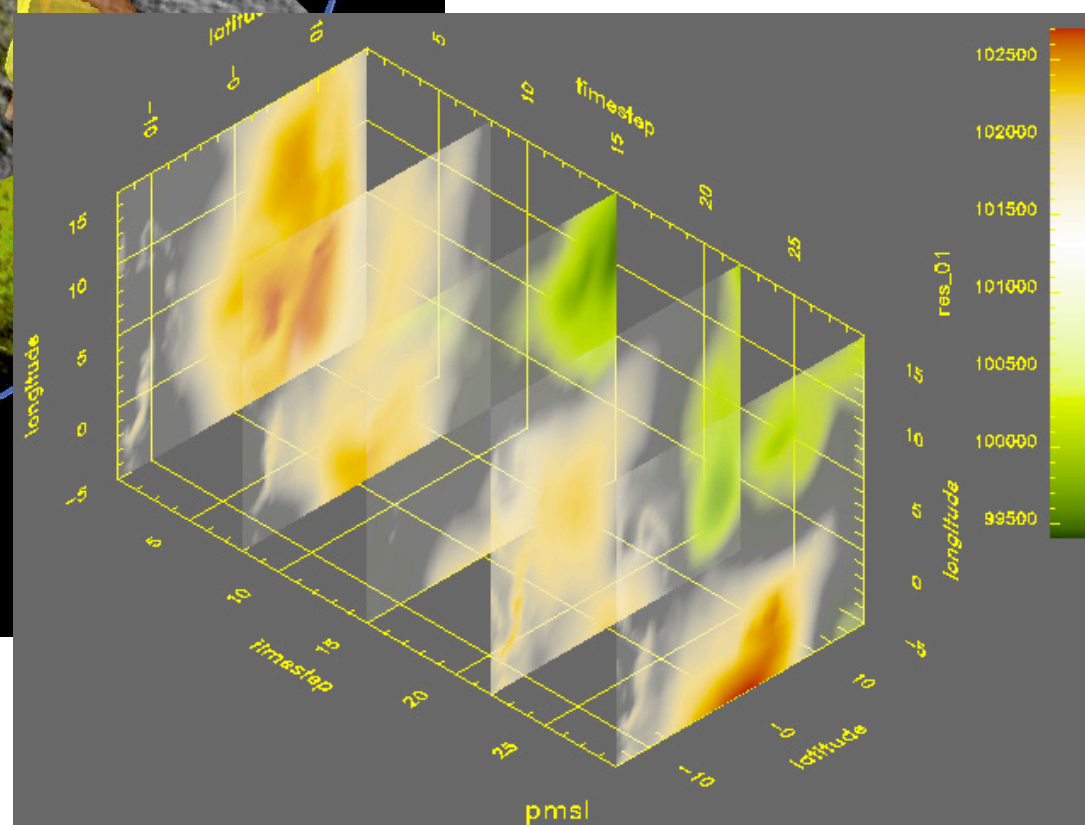
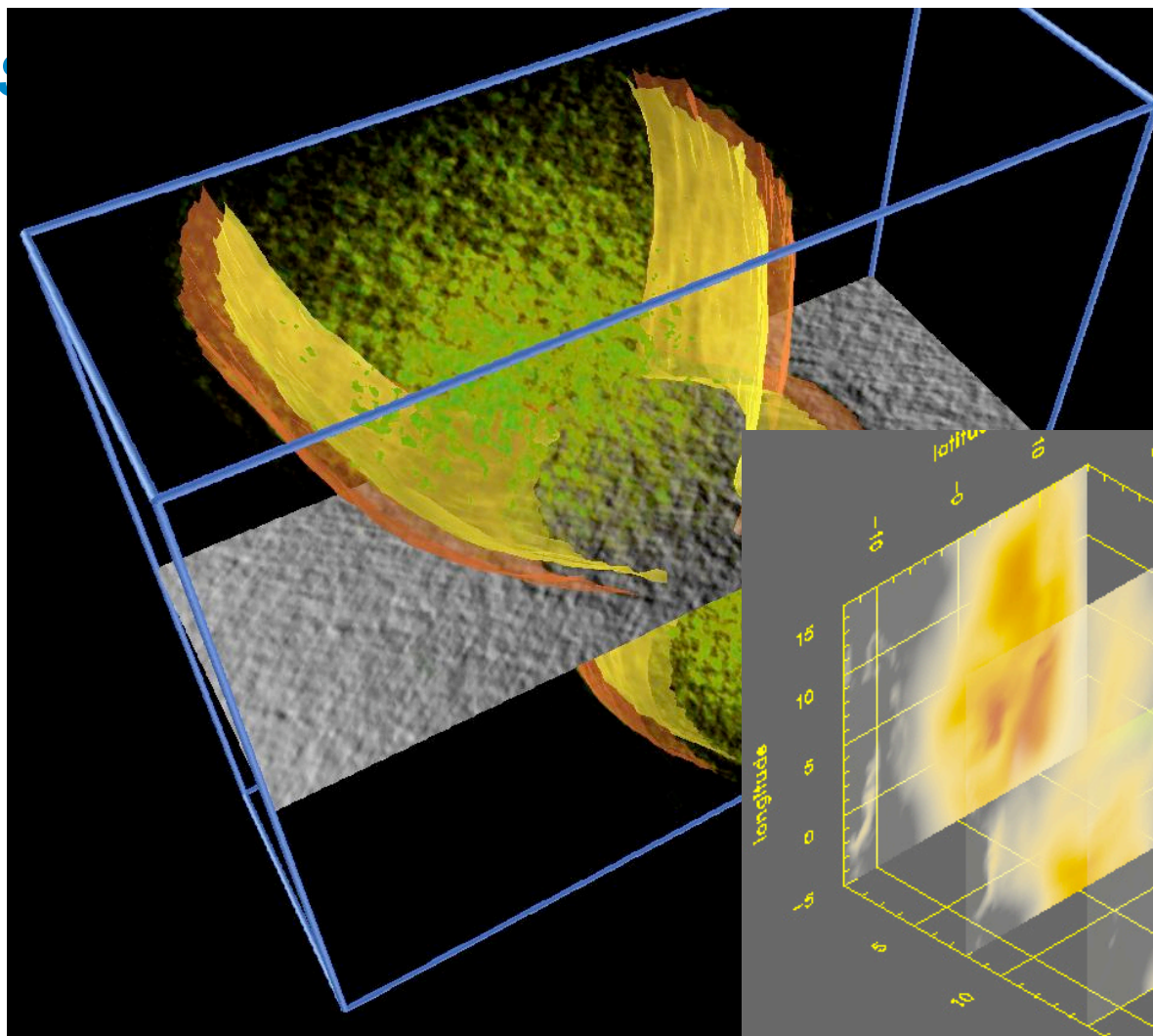
- Confounding circumstances
 - Compute is far away, expensive, batch
 - Storage is distant as well
 - *Datasets are very large*
 - *Disk speed and network bandwidth are constraining*
 - Workstation and display pixels are local
 - *And these are limited in capacity*
- Exploring results is challenging
- Data volume example
 - 32K procs each handling 29x29x29 cells
 - *928 x 928 x 928 cells*
 - 751 time steps, 21 variables
 - *30 GB HDF5 file per step, 22 TB total*

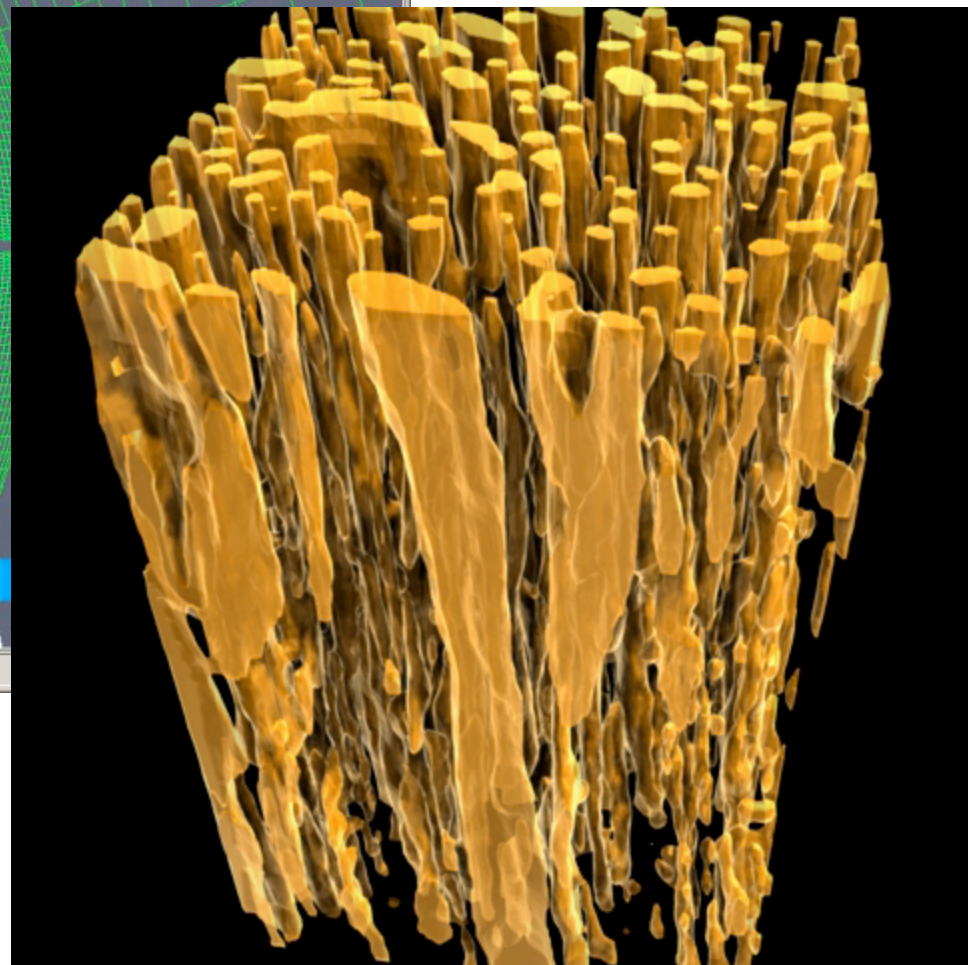
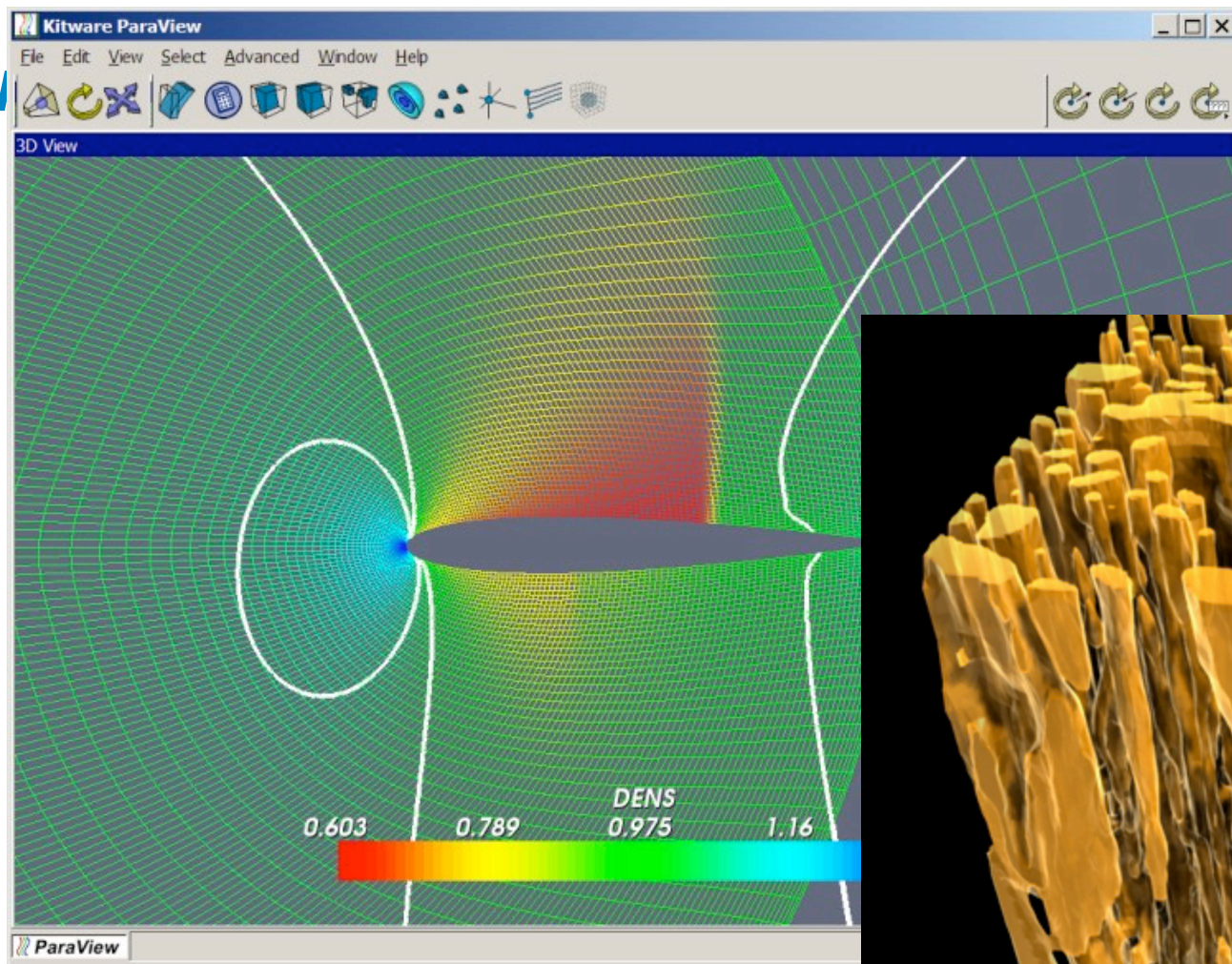
All Sorts of Tools

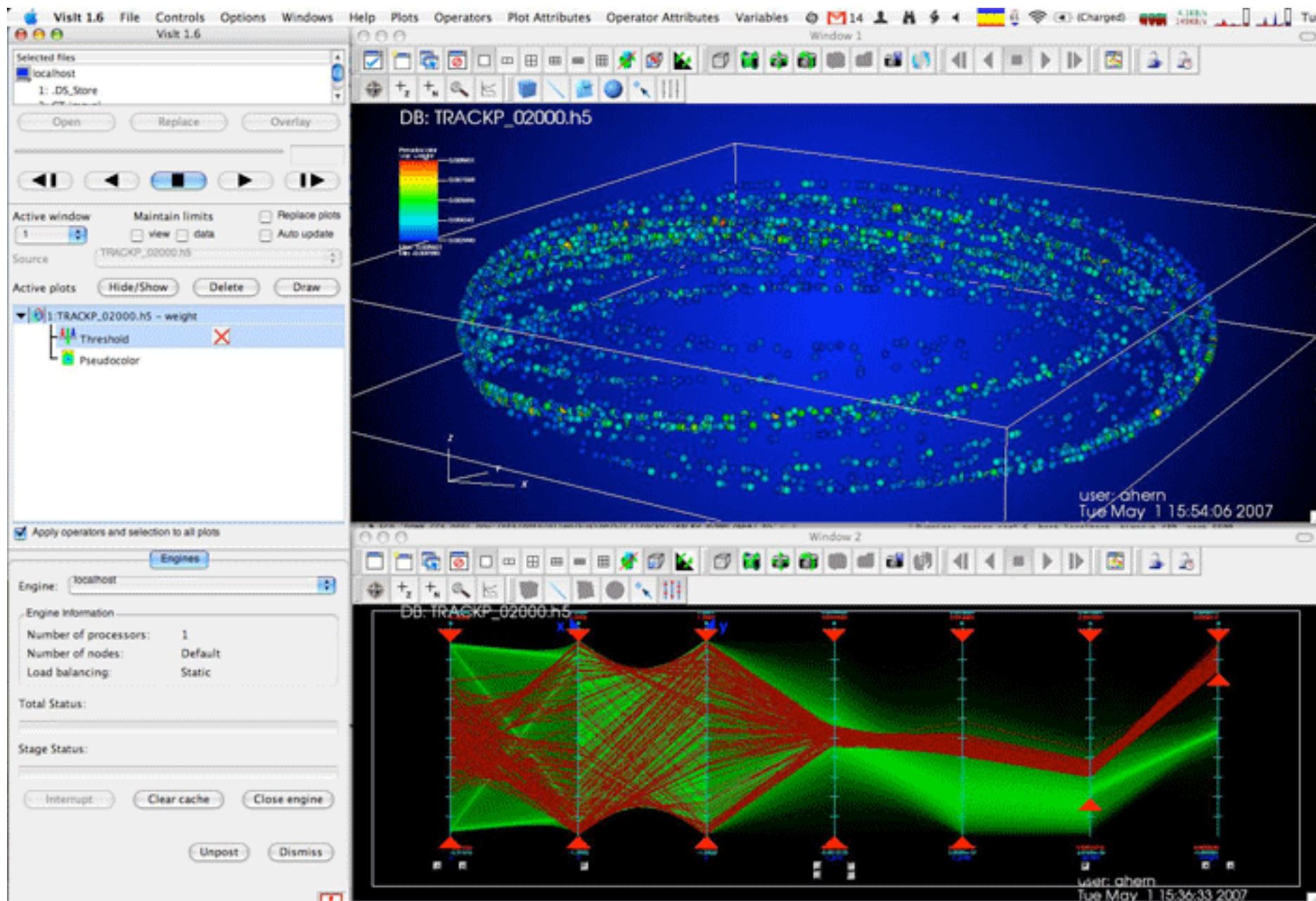
- Visualization Applications
 - VisIt
 - ParaView
 - EnSight
- Domain Specific
 - PyMol, RasMol
- APIs
 - VTK: visualization
 - ITK: segmentation & registration
- GPU performance
 - Scout: GPGPU acceleration
 - vl3: shader-based vol ren
- Analysis Environments
 - Matlab
 - Parallel R (ORNL)
- Utilities
 - GnuPlot
 - ImageMagick
- Visualization Workflow
 - VisTrails



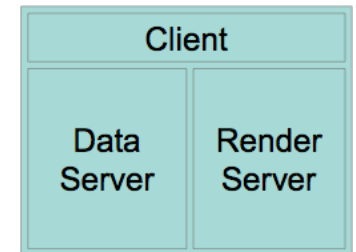








ParaView Overview



- Parallel Visualization Application
- Open source
- VTK + Tcl
- Python scripting
- Interactive and batch
- About

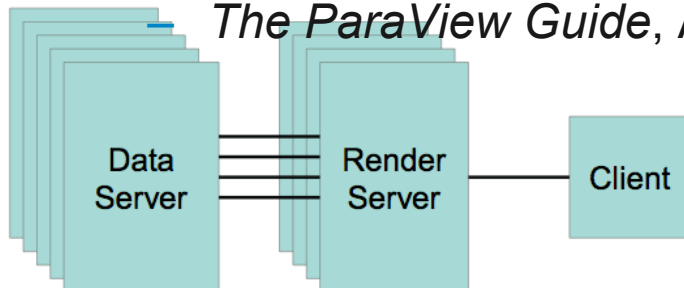
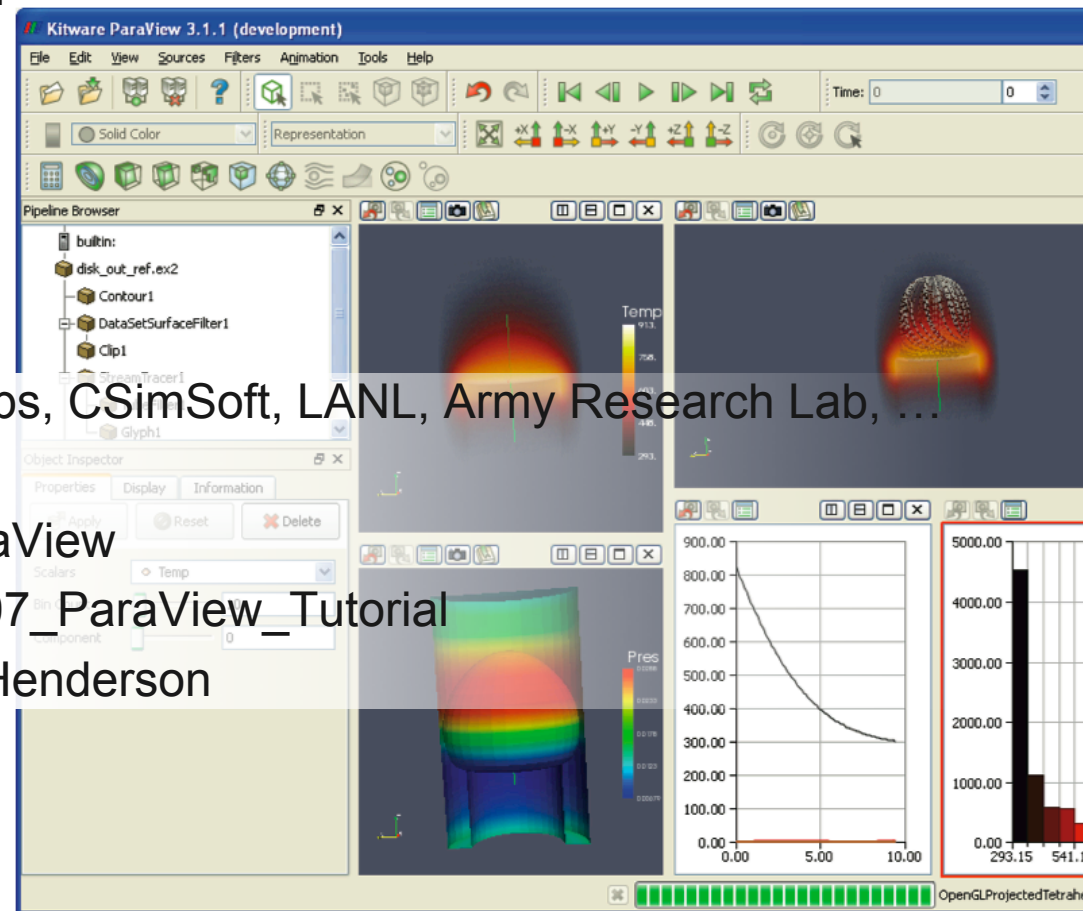
— Kitware, Sandia National Labs, CSimSoft, LANL, Army Research Lab, ...

— <http://www.paraview.org>

— <http://paraview.org/Wiki/ParaView>

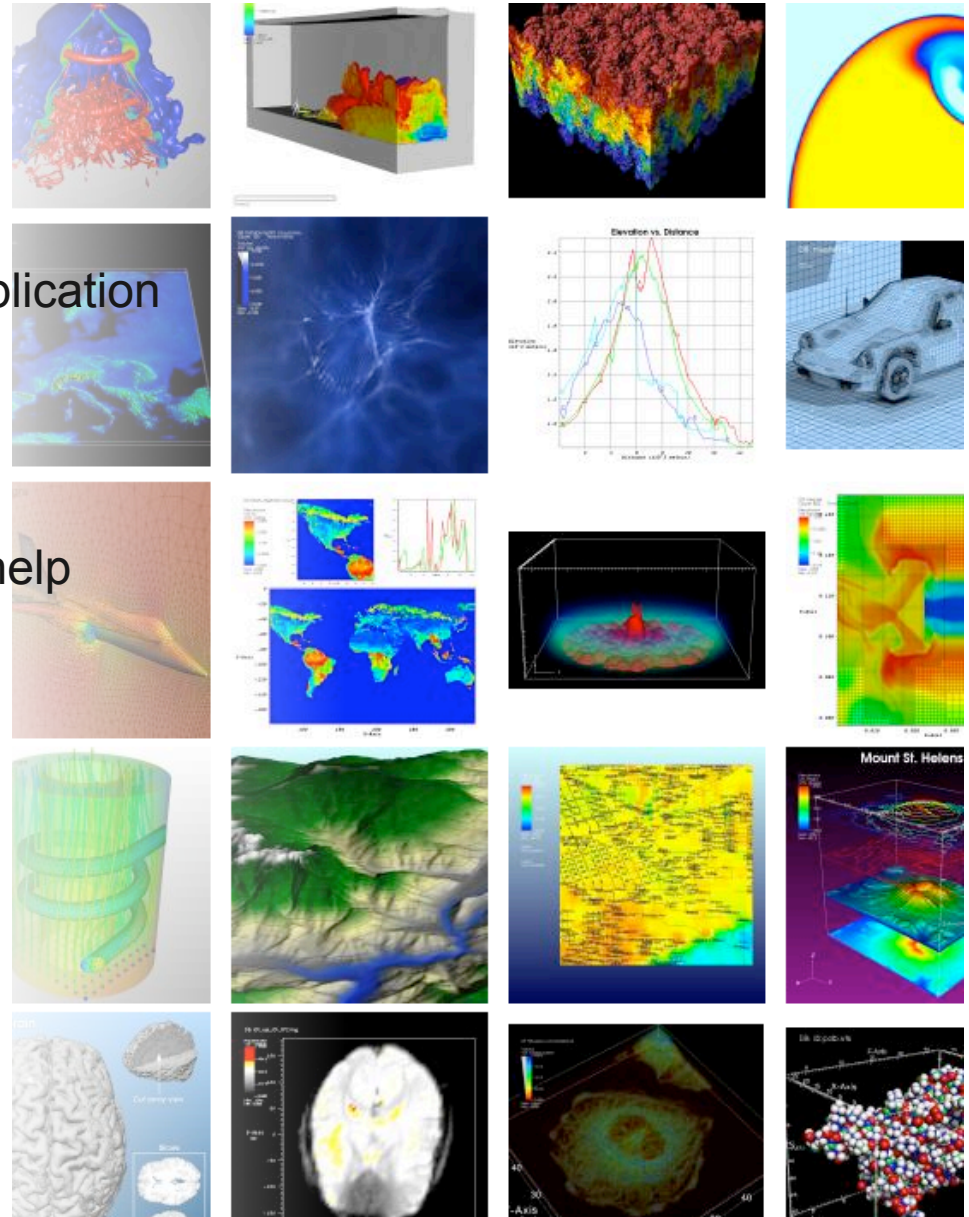
— http://paraview.org/Wiki/SC07_ParaView_Tutorial

— *The ParaView Guide*, Amy Henderson



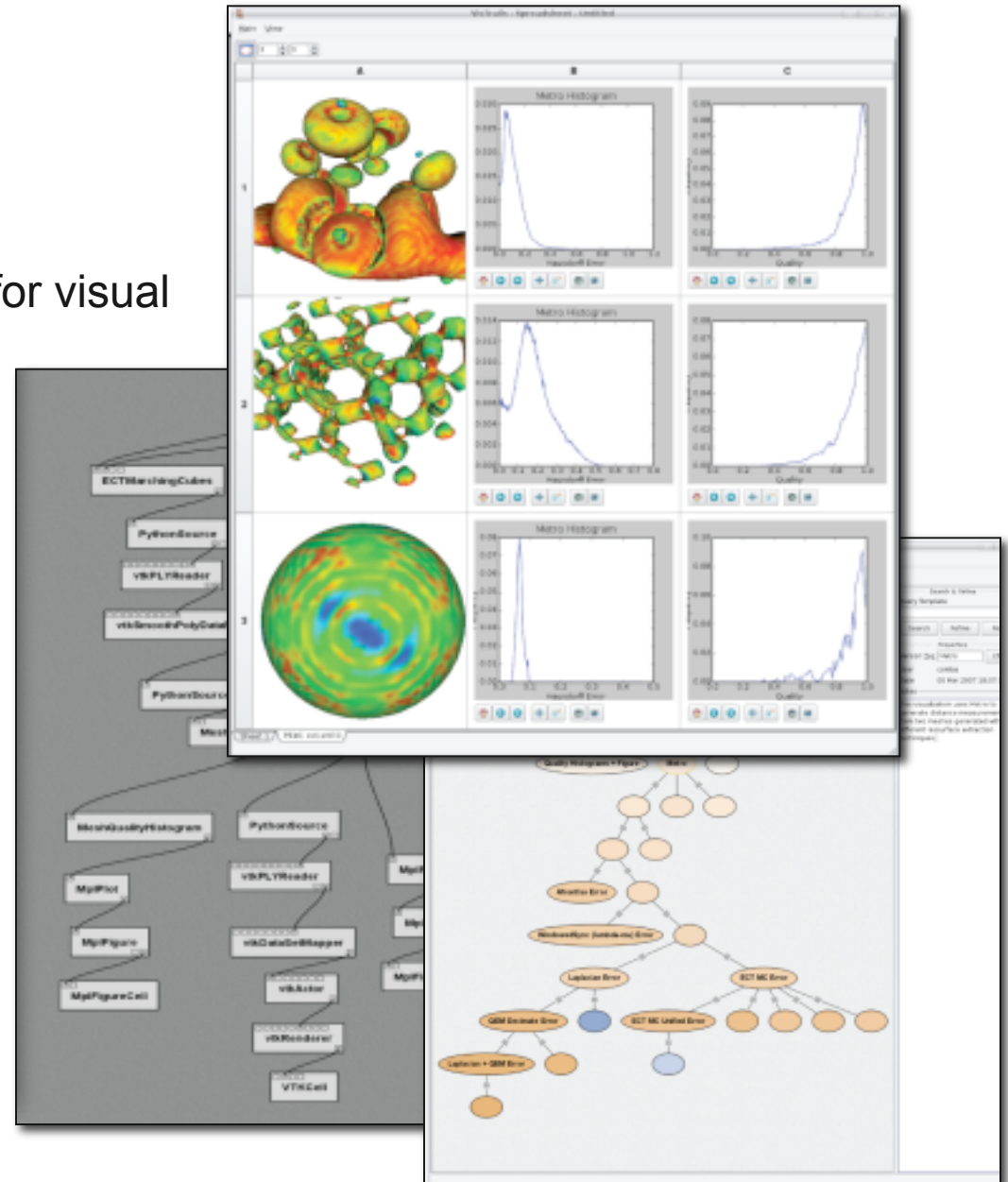
Visit Overview

- Parallel interactive visualization application
- About
 - DOE ASCI
 - <https://www.llnl.gov/visit>
 - Manuals, tutorials, application help



VisTrails

- Scientific workflow management for visual data analysis
- Visual programming
- Construct and execute pipelines
 - VTK, ITK, and Matplotlib
- History tree captures provenance
- Visualization spreadsheet
- About
 - <http://www.vistrails.org>

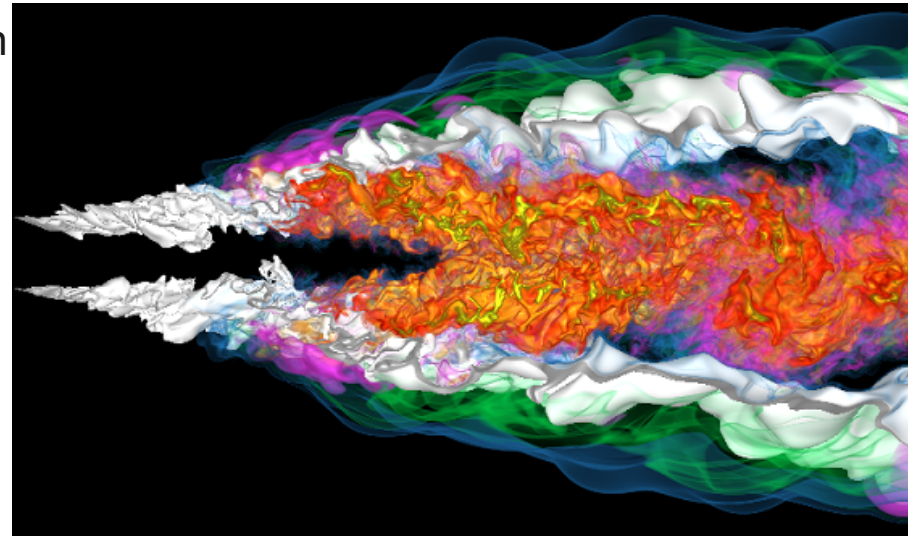


In situ analysis and data reduction

- Incorporate analysis routines into the simulation code
 - operate on data while it is still in memory
- Potential for significant reduction the I/O demands
 - application scientist identifies features of interest
 - compress data of less interest

Here, the feature of interest is the mixture fraction with an **iso-value of 0.2 (white surface)**. Colored regions are a volume rendering of the HO₂ variable (data courtesy J. Chen).

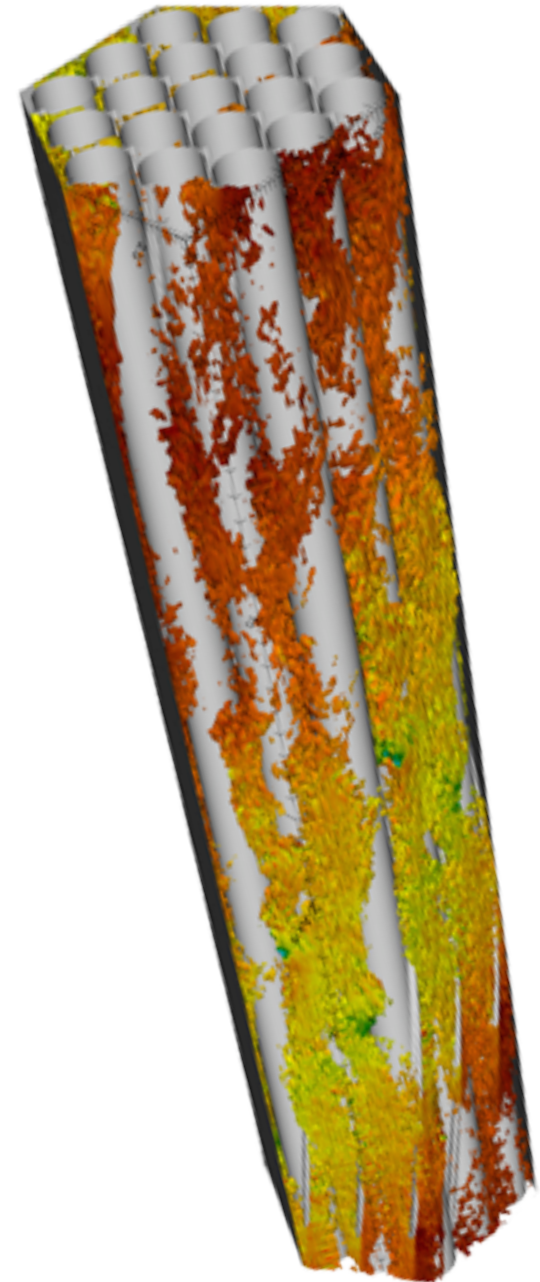
By compressing data more aggressively the further it is from this surface, we can attain a compression ratio of 20-30x while still retaining full fidelity in the vicinity of the surface.



C. Wang, H. Yu, and K.-L. Ma, "Application-driven compression for visualizing large-scale time-varying volume data", IEEE Computer Graphics and Applications, accepted for publication.

Nuclear Reactor Simulation

- Preliminary studies
 - 4.5 million elements
 - 7 variables per element
 - 20 K timesteps
 - Total data produced 2.5 TB
- Science runs
 - 3 – 4 runs with 120 million elements
 - Several runs at $\frac{1}{2}$ and $\frac{1}{4}$ resolution
 - 90 K timesteps
 - Total data produced 900TB – 1.2 PB



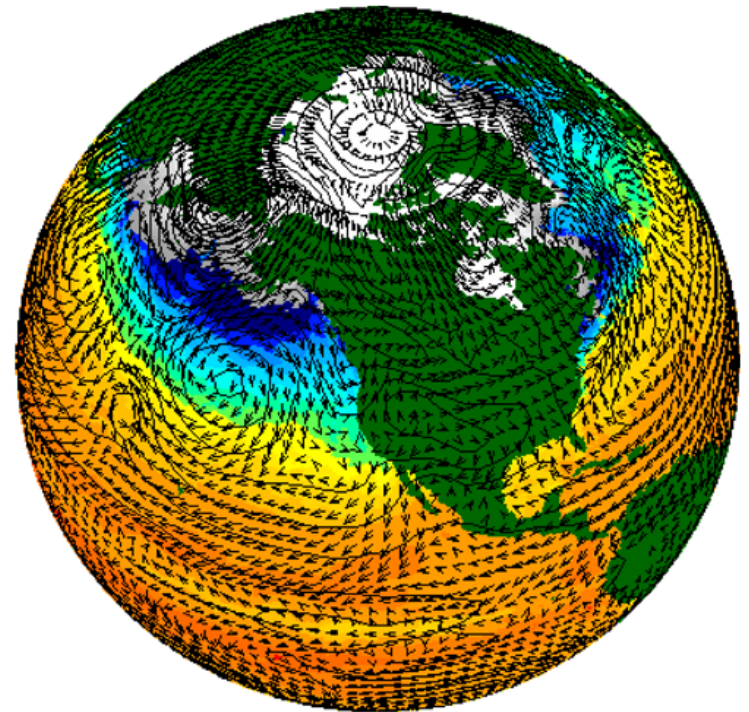
Climate Modeling

■ Preliminary studies

- 50-100 with 3 million grid points (1 M atmosphere, 2 M ocean)
- 100 variables per grid point (30 vectors, 70 scalars)
- Simulating 5 - 10 years of climate
- Total data produced 30 -124 TB

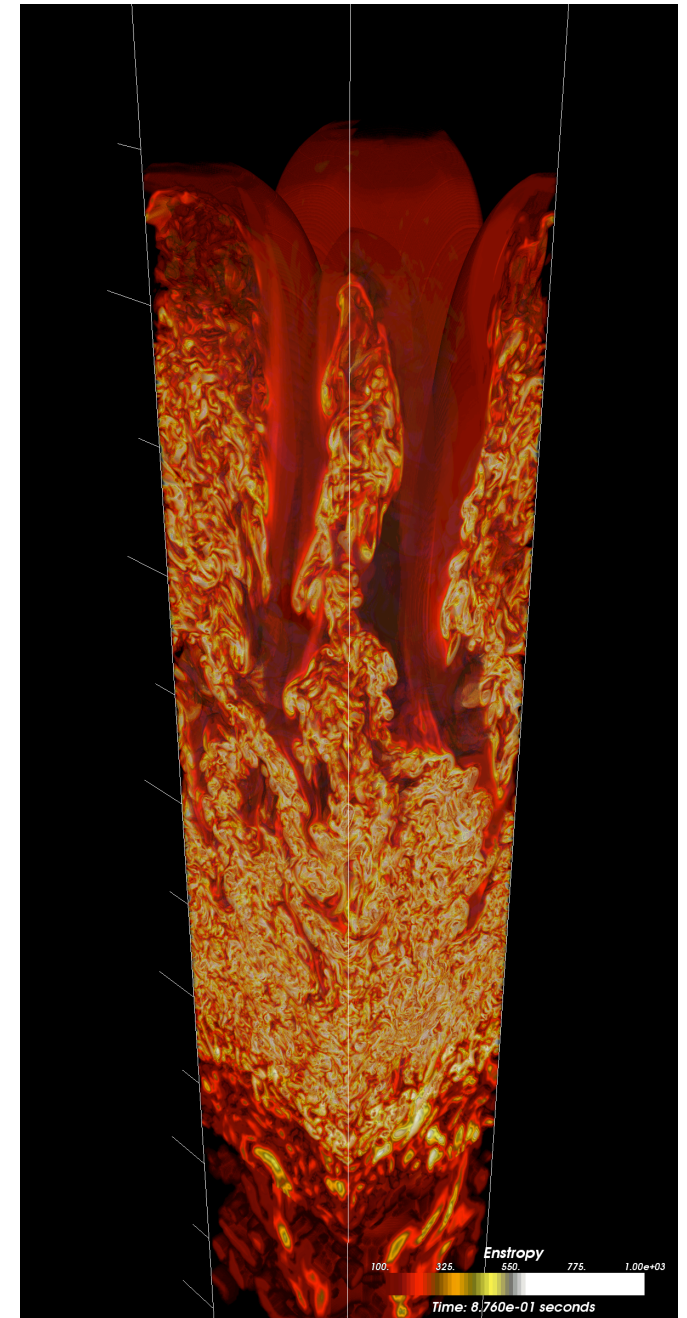
■ Science runs

- 50 runs with 6 million grid points
- Simulating 100 years of climate
- Total data produced 1.2 PB



Astrophysics

- Preliminary studies
 - ~80 with 67 M grid points
 - ~5 with 536 M grid points
 - 6 variables (1 vector, 3 scalars)
 - ~1800 time steps
 - Total data produced 78 TB
 - Science run*
 - $1024^2 \times 4096$ grid points
 - 6 variables (1 vector, 3 scalars)
 - ~1800 time steps
 - Total data produced 48 TB
- * 3-5 times bigger allocation is needed



Analysis/Visualization Questionnaire – Overview

- Do you have preferred computational platform?
- What are your dataset sizes?
 - Do you have checkpoint files and analysis files or is everything together?
- How long do your simulations run? (e.g. wall clock time)
 - Is the result a time series?
 - How many files does that produce?
- Do you do your analysis local or using remote resources?
 - Why?
- How long do you spend on analysis, what is the fraction of compute versus human?

A/V Q – Your I/O footprint

- How much of your simulation time is I/O? (e.g. 10%)
- Do you do data reduction (e.g. convert from double to float during I/O, subsample data, ...)?
 - Why?
- What are your transfer rates to disk from simulation? (e.g. bandwidth)
- What are your transfer rates from disk for analysis? (e.g. bandwidth)

A/V Q – Your Goals

- What do you look to get out of analysis process?
- What analysis tools are you currently using?
 - What are the limitations?
- Do you do real-time exploration or batch processing?
 - What is the role of real-time exploration?
 - Batch?
 - Percentage of your analysis time spent in either mode?
- Do you look at images, movies or graphs?
 - What is role of each (e.g. graphs for science, images publications, movies for talks)